Perspectives on Large Eddy Simulations for Sprays: Issues and Solutions

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Abstract
A review of the Large Eddy Simulations (LES) methodology is presented in the context of sprays. Issues related to the modeling of both the drop interaction with the carrier flow and of the interaction among drops are discussed. Appropriate Direct Numerical Simulations (DNS) for use as precursors to LES, and the extraction of Subgrid Scale (SGS) models are both described. Particular attention is devoted to LES aspects which are different from those of single-phase flows. These include the correct portrayal of the drop interaction with small turbulent scales, the modeling of SGS stresses, SGS heat and SGS species fluxes, and the accurate representation in the carrier flow equations of the source terms associated with the presence of the drops. Recommendations for future work are also offered.

Introduction

The mathematical description of turbulent drop laden flows is one of the challenges of contemporary multiphase flow research. This is because additional to the still unresolved complexities associated with single phase turbulent flows, the interaction between drops and flow, and among drops introduce modeling difficulties that are so far unsolved. Past modeling approaches included modifications of the $k - \varepsilon$ methods, based on the Prandtl length hypothesis, with the drops described either in a Lagrangian manner of in an Eulerian way, and also Monte Carlo methods whereby it is assumed that a subset of the total number of drops is representative of the entire ensemble, thus eliminating the need to follow a prohibitively large number of drops. More recently, the method of Large Eddy Simulations (LES) has received increasing attention because of its potential for efficiently describing the interaction between drops and the carrier gas. This method is the subject of this review paper.

The LES formalism is based on a conceptual partition of scales. Since resolving all scales of a turbulent flow is presently, and in the foreseeable future, impossible due to computer memory and computational time constraints, instead, one divides the problem into two tractable parts, the small scales and the large scales, and then connects the latter to the former through modeling. Information about small scale behavior may be obtained either from experimental data or from Direct Numerical Simulations (DNS). Although experiments with liquid drops in shear and mixing layers do exist [1], [2], [3], [4], [5], [6], [7], results reporting vapor distributions from evaporating drops are restricted to few studies [8], [9]. Because the observational data does not currently allow a basic understanding of evaporating/combusting sprays, this review will focus on the DNS/LES combined methods.

In DNS the small scale problem is completely resolved for a domain that is smaller than the macroscopic scale of interest, and for the lower end of the turbulence regime. The connection between small and large scales is made by using the DNS database to extract the essence of turbulent small scale behavior through Subgrid Scale (SGS) models (this process has been termed an *a priori* study); a detailed explanation of this protocol is given below. One must distinguish between constant-coefficient SGS models that are dependent on the geometric configuration and dynamic SGS models that are independent of the configuration. Obviously the latter are preferable to the former because of their wider range of applicability to explore a variety of configurations. The large scales are solved by spatially filtering (i.e. averaging) the original equations to remove the small turbulent scales that cannot be solved exactly, thereby obtaining the LES equations. In the LES equations, the correlations resulting from filtering (which contain the effect of the turbulent scales) are then replaced with the SGS models. This procedure is based upon the assumption that the small turbulent scales behave essentially in the same manner at the low and high end of the Reynolds number in the turbulent regime, and reintroduces in the equations the small scale effect that would otherwise be lost. Studies conducted with the LES equations are called *a posteriori* investigations. It is by now recognized that even well-behaved *a priori* models may not retain their good comportment in *a posteriori* studies because these latter embed the additional aspect of length scale interactions that lack in the former. Therefore, among several possible SGS models, only a subset, or none, may be computationally stable and be considered for the next and last step of model development which is that of model validation with data.

This paper is organized as follows: First, a critical review of existing LES investigations is presented with the goals of understanding the state of the art and of identifying possible deficiencies necessitating further studies. This is followed by separate discussions on each of the issues that may have been identified during the critical review. Finally, conclusions are offered on the near-future prospects of LES in the context of sprays.

Background on LES

General concepts

To apply the DNS/LES protocol in which SGS models are derived from the former and used in the latter, the same equations must be solved in both DNS and LES. In the DNS/LES protocol, the conservation equations are solved for the carrier flow in an Eulerian frame whereas those for the drops are solved in a Lagrangian frame. An Eulerian/Eulerian representation is not possible in DNS without further assumptions (and therefore not feasible in an *a posteriori* LES, although possible in a LES where an already exiting dynamic SGS is used). This is because the drop number density (n) equation (i.e. the continuity equation for the condensed phase) cannot be solved without an effective drop diffusion term, being mathematically too stiff without it; and this term is unknown prior to solving the equations. (A comprehensive discussion of the effective diffusion term that must be added to the particle number density and momentum Eulerian equations to avoid this singularity appears in Tong and Wang [10]. It is pointed out that this numerical diffusion term is effectively equivalent to the necessary smoothing of the particles contribution in the Eulerian/Lagrangian approach; see below.) To use the DNS/LES protocol, the same DNS Eulerian equations must be spatially averaged in order to obtain the corresponding carrier flow LES equations. In the LES based on the Eulerian/Lagrangian representation, the same drop equations are solved as in DNS because it is meaningless to spatially average equations in a Lagrangian frame; however, as will be discussed below, in the LES the drop equations have a different meaning than in the original DNS.

A fundamental difficulty arises, however, in the formulation of the DNS equations for a flow containing the very large number of drops (e.g. $\sim O(10^6)$) necessary to perform meaningful statistics for extracting SGS models. This difficulty is associated with the fact that, due to computer memory and computational time constraints, the exact equations inside the drops and in their immediate vicinity cannot be resolved even for a small domain and for a relatively small (~ 400) initial Reynolds number, Re^0. The strategy for making the problem computationally tractable is to assume the drops much smaller than the Kolmogorov scales, and treat them as point forces and sources (e.g. [11], [12], [13], [14], [15], [16]). This means that the force on the drop in the momentum equations (both carrier and drops) is already modeled according to well-validated models. Correspondingly, the vapor emission from the drops is also modeled according to well-established and validated models [17]. Liljegren [18] noted that this point force/source assumption leads to loosing the effect of particles on the fluctuating kinetic energy of the carrier flow to leading order. Although some investigators are reluctant to calling such studies DNS, this is only a matter of semantics and current alternatives do not exist for a large number of drops. Glowinski et al. [19] discuss state-of the-art methods in DNS for flows carrying a small number of solid particles where each particle's motion and that of the flow around it is resolved using a weak statement of the momentum equation and where the no-slip condition at the particle surface is enforced by using Lagrange multipliers which act as additional constraints. These methods are called *domain-embedding* methods, and have been applied so far to incompressible flows only. Moreover, since the fluid-particle motion is only treated implicitly through a combined equation of motion, thus eliminating the need to calculate mutual forces, this method holds poor prospects for evaporating drops for which the knowledge of the conditions at the drop surface are essential to enable the calculation of the mass flux. Therefore, although the formulation of the evaporating drops as finite volumes is mathematically feasible, in the context of a very large number of drops it is currently computationally unfeasible.

Another difference in formulation arises between the LES procedure with drops treated as point forces/sources and drops treated as finite volumes due to the interpretation of spatial averaging. The concept of spatial averaging is easily defined in single-phase flows where the DNS/LES formalism originated, but in the context of two-phase flows special care must be exercised to perform a meaningful average. Basically, one can no longer formally average the carrier flow equations over the entire domain because the fluid is not present at locations where the drops reside, as lucidly discussed by Liljegren and Foslein [20]. Even for initially dilute two-phase flows (i.e. small drop volume fraction, $\sim 10^{-3} - 10^{-4}$) the distinction could be important because although on average the mixture will remain dilute, due to preferential concentration effects (see [21], [12], [22], [16]) there will be local regions where the drop volume fraction will be considerably larger. With this concern, Liljegren and Foslein [20] used conditional averaging concepts developed for granular flows [23] to derive equations for the fluctuating kinetic energy in both phases. Basically, to separate the phases, the averaging must then be performed only in the spatial region containing that phase, this being the condition for averaged terms to possibly be non nul.

In the following discussion studies with negligible and substantial condensed phase volume fraction will be considered.

SGS models

SGS models are the crucial component of LES. As explained earlier herein, the role of SGS models is to reintroduce into the spatially filtered LES equations the missing influence of the small turbulent scales; the small scales are missing in the LES equations precisely because they have been removed by the filtering process, since they cannot be resolved in a flow that encompasses large scales. In two-phase flows, an additional difficulty arises because in a LES it is only the filtered (i.e. large scale) solution that is available, yet the drops are profoundly influenced by the small scales (which are not known from the LES solution); neglecting this phenome non would be omitting one of the most important aspects of two-phase flows. To include this crucial feature of two-phase flows, Okong'o and Bellan [24] modeled the unfiltered flow field at the drop locations using the LES flow field, and have shown that the model thus obtained is very accurate, as will be discussed below.

Several types of SGS models are potentially possible [24], the most well-known being the Smagorinsky (SM), the Gradient (GR) and the Scale-Similarity (SS) models. However, for two-phase flows with single-component drops Okong'o and Bellan have shown [24] that only the GR model (e.g. Liu et al. [25]) and the SS models [26] are viable because the SM model [27] does not correlate at all with the results from the DNS database. All these models are obtained from a database by assuming the functional form of the SGS viscous stresses, SGS molar and SGS heat fluxes, and finding a proportionality constant through comparison with the database. The difference between constant-coefficient and dynamic modeling is that the functional form of the latter is more complex and adjusts itself as a function of time to the evolution of the flow. Specifically, the GR model assumes that the SGS viscous stresses, SGS molar and SGS heat fluxes can be modeled as a function of a tensor which is the product of the gradient of the particular dependent variable with the velocity gradient, as follows

$$\tau_{ij} = C_G \Delta^2 \frac{\partial \widetilde{u}_i}{\partial x_k} \frac{\partial \widetilde{u}_j}{\partial x_k} \tag{1}$$

$$\theta_j = C_G \Delta^2 \frac{\partial \overline{T}}{\partial x_k} \frac{\partial \widetilde{u}_j}{\partial x_k} \tag{2}$$

$$\eta_j = C_G \Delta^2 \frac{\partial \widetilde{Y}_V}{\partial x_k} \frac{\partial \widetilde{u}_j}{\partial x_k} \tag{3}$$

where Δ is the filter size, C_G is the proportionality constant to be determined from comparison with the database in constant-coefficient SGS models, τ_{ij}, θ_j and η_j are the SGS stress tensor, SGS heat flux and SGS mass flux of the evaporated species, respectively; $\widetilde{u}_i$ is the i component of the Favre averaged flow velocity, x_k is the k^{th} coordinate, $\overline{T}$ is the (unweighted) averaged temperature, and $\widetilde{Y}_V$ is the Favre averaged mass fraction of the evaporated species.

The SS model assumes that most of the exchange between flow scales occurs between the lower end of the large scales and the higher end of the small scales, and that these scales behave in a self-similar manner. Therefore, the SS protocol introduces a second filter, $\widehat{\Delta} \geq \Delta$ (filtering at level $\widehat{\Delta}$ is unweighted), typically twice the size of the first filter, and the SGS fluxes are thus modeled as being proportional to the difference between the refiltered product of the already filtered quantities and the product of the refiltered quantities:

$$\tau_{ij} = C_S \left(\widehat{\widetilde{u}_i \widetilde{u}_j} - \widehat{\widetilde{u}}_i \widehat{\widetilde{u}}_j \right) \tag{4}$$

$$\theta_j = C_S \left(\widehat{\widetilde{u}_j \overline{T}} - \widehat{\widetilde{u}}_j \widehat{\overline{T}} \right) \tag{5}$$

$$\eta_j = C_S \left(\widehat{\widetilde{u}_j \widetilde{Y}_V} - \widehat{\widetilde{u}}_j \widehat{\widetilde{Y}}_V \right) \tag{6}$$

where C_S is the proportionality constant in constant-coefficient models.

Since the proportionality constant for both constant-coefficient GR and SS models is generally smaller than the theoretical value (i.e. $C_R = 1/12$ and $C_S = 1$, meaning perfect correlation), most dynamic SGS models (where C_R and C_S are no longer constants) rely to a certain extent on a contribution from the SM model to insure that the total dissipation is accurately modeled. The SM model is

$$\tau_{ij} = -2 C_{SM} \Delta^2 \sqrt{\widetilde{S}_{kl} \widetilde{S}_{kl}} \left(\widetilde{S}_{ij} - \frac{1}{3} \widetilde{S}_{kk} \delta_{ij} \right) \tag{7}$$

$$\widetilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} \right) \tag{8}$$

$$\theta_j = -\frac{C_{SM} \Delta^2}{\mathrm{Pr}} \sqrt{\widetilde{S}_{kl} \widetilde{S}_{kl}} \frac{\partial \overline{T}}{\partial x_j} \tag{9}$$

$$\eta_j = -C_{SM} \Delta^2 \sqrt{\widetilde{S}_{kl} \widetilde{S}_{kl}} \frac{\partial \widetilde{Y}_V}{\partial x_j} \tag{10}$$

where C_{SM} is a model constant, $\widetilde{S}_{ij}$ is the rate-of-strain tensor for the filtered velocities and Pr is the Prandtl number. However, for a drop laden shear layer Okong'o and Bellan [24] found that this additional complication may be neither desirable, because the SM model correlated very poorly with the database, nor necessary, because the proportionality constant for the constant-coefficient GR and SS models alone was remarkably large showing an excellent correlation and representation of the dissipation.

Since the formulation of SGS models using DNS databases is currently at its inception, most existing two-phase flow LES studies are based upon assumed SGS models emulating those found in single-phase flows.

Existing two-phase flow LES

Currently available LES investigations have in common semi-empirical SGS models, and in this respect are similar to other simulations of turbulent flows using either Prandtl mixing length, Reynolds stresses or $k - \varepsilon$ simulations. For example, Deutsch and Simonin [28] use a two-fluid Eulerian formalism with the condensed phase having a non-negligible volume fraction and assume that the SGS flux is proportional to the gradient of the dependent variable, similar to the Prandtl mixing length hypothesis. Particles moving through a homogeneous turbulent shear layer fluid without affecting it (having assumed negligible volume fraction and interphase momentum transfer) were simulated by Simonin et al. [29]; this type of study where the particles do not affect the flow is called a 'one-way' coupling investigation. The particle motion was followed in a Lagrangian way and the fluid was simulated by LES using a single-phase SM model with the proportionality constant determined from comparison with experimental data in decaying isotropic turbulence. Comparison between these predictions and those based on a solution of equations for the particle kinetic stress and for the fluid-particle velocity correlations using a second-order closure model of the particle fluctuating motion, were in agreement. Also a one-way coupling study was presented by Wang and Squires [30] describing a vertical channel incompressible flow where the solid particle motion was governed by both drag and lift and the Germano dynamic approach [31] was used to determine the SGS model. In the dynamic approach, the concept is to use the larger, resolved scales to calculate the model coefficient during the course of the calculation. Specifically, in a dynamic model a second filter, called 'test' filter, is defined, slightly larger than the grid filter ($\widehat{\Delta}/\Delta = 2^{2/3}$ in [30]) and the filtered equations are refiltered to yield subtest-scale stresses, heat and mass fluxes which are the sum of the corresponding resolved quantities and the corresponding SGS quantities. For the stresses, this relationship is called the Germano identity whose form for compressible flows is (ρ is the density)

$$\widehat{\overline{\rho}}\mathcal{L}_{ij} = \widehat{\overline{\rho}}T_{ij} - \widehat{\overline{\rho}\tau_{ij}} \qquad (11)$$

and which relates the resolved stress $\mathcal{L}_{ij}$ to the SGS stresses, τ_{ij}, and the subtest-scale stresses, T_{ij}, both of which need to be modeled. For any τ_{ij} and T_{ij} models mathematically expressed by a functional form multiplied by a proportionality coefficient, such as presented above for constant-coefficients models, substitution of these models into eq. 11 allows the dynamic determination of the model coefficients as the LES proceeds; this determination is based upon the information (i.e. the energy) contained in the smallest resolved scales. Since the system of equations is overdetermined, the usual procedure is actually to find an approximate value of the proportionality coefficient from the constraint of minimizing the error between the unknown solution and its approximation by a least-square fit. Particle deposition rates predicted by Wang and Squires [30] agreed reasonably with those from DNS simulating the same situation, thereby giving credence to their model. Moreover, in a similar calculation using $\widehat{\Delta}/\Delta = 2$ [32], visualization of particles number density and particle preferential concentration agreed also with observations. Two-phase channel flow was similarly investigated by Uijttewaal and Oliemans [33] using the one-way hypothesis, and the SGS model was based on the constant-coefficient SM relationship. Their rate of deposition results were also in good agreement with observations showing that perhaps this type of problem is somewhat insensitive to the SGS model.

Shear flows laden with solid particles were studied by Wang and Squires [34] in incompressible mixing layers and by Yeh and Lei [35] in homogeneous flows. In both of these investigations, SGS single-phase models were used since the flow was assumed unmodified by the presence of particles. Both of these studies yielded predictions in reasonable agreement with experimental measurements for similar configurations and regimes.

To this author's knowledge, the first 'two-way' coupled LES, whereby the particles influence the flow, was performed by Oefelein and Yang [36] in the context of supercritical drops. The chosen two-dimensional geometry was that of the mixing layer with two hydrogen streams framing a liquid oxygen drop spray. The point force/source approximation was used to follow statistically significant samples of drops on their trajectories. The flow was compressible and various types of SGS models were used to model correlations in the filtered equations, although all of the models originated from single-phase flows and there was no attempt to account for the local interaction between drops and turbulent fluctuations. This was consistent with the assumption that the drops are smaller than the Kolmogorov scale at all times, and thus the interactions between drops and flows can be considered dominated by instantaneous laminar fluid dynamics. The SGS momentum and species fluxes were modeled using the Erlebacher et al. [38] model with a combination of constant-coefficient SS and SM models. The results showed significant coupling between drops and flow, and increased sensitivity to both SGS fluctuations and large scale coherency with increasing pressure. Pannala and Menon [37], however, question the methodology of accounting for a limited size range of drops, above a cut-off size, as it is inherently done in a statistical approach. They explain that the drops which are unaccounted for become effectively fully vaporized and the resulting vapor is fully mixed with the oxidizer bypassing the realistic time delay necessary for these processes to occur. To palliate this inaccuracy, Pannala and Menon [37] propose that beside tracking the larger drops in the same, Lagrangian manner as in [36], one should track the smaller than the cut-off size drops in an Eulerian manner, through a subgrid model that will include the effects of the small drops within the LES grid. Therefore, in this incompressible flow formulation, the Linear Eddy Mixing (LEM) model of Kerstein [39], [40] is enlarged to effectively account for a (minuscule) subgrid void fraction, and separate mass conservation equations are written for gas and drops. In the spirit of the LEM whereby the convective part of the subgrid is separated from the transient one and modeled by turbulent stirring, both of the mass conservation equations contain only transient and source/sink terms. The source terms for the gas conservation equation express contributions due to vaporization of the drops tracked on the supergrid and on the subgrid. The liquid conservation equation has one source term expressing the contribution of the supergrid to the subgrid liquid phase and a sink term representing the vaporization of the subgrid drops. Since the Eulerian equation for the subgrid drops is not presented, it is unclear how the authors calculate the subgrid drop number density and therefore the subgrid source of vapor. Moreover, since Kerstein's model was derived in the context of single-phase flow, its validity for two-phase flow situations remains to be determined. The findings of Pannala and Menon [37] were that the subgrid drops become increasingly important with increasing cut-off size.

Clearly, there are several issues that are so far unresolved for conducting a realistic two-phase flow LES. First, none of the above cited LES studies uses a SGS model derived either from two-phase flow experiments or from a two-phase flow DNS. Second, there is an uncertainty as to the number of drops which should be followed in a LES compared to the number of drops present in the situation that is emulated. Third, whereas the majority of LES investigations ignored the effect of the particles on the flow, it seems that this aspect is important even for dilute flows; however, the manner in which one could model the drop interaction with the small turbulent eddies is not immediately clear. Finally, the stability of SGS models in LES studies is an open subject yet unexplored.

DNS of two-phase anisotropic, inhomogeneous 3D shear flows

The scarcity of extensive and fundamental experimental data for two-phase flows with substantial mass loadings and phase change renders two-phase flow DNS studies prominent for deriving SGS models. Among all DNS studies with particles, only those that are both in anisotropic and inhomogeneous flows will be discussed because of their relevance to sprays. Further eliminated are those DNS studies limited to laminar flows because they are irrelevant to the extraction of SGS models. The particular focus is here on shear flows because they provide one of the building blocks for studying sprays. Despite their interest as a fundamental research tool, two-dimensional mixing layers are also omitted in this review since they cannot evolve the truly turbulent features necessary for SGS model development.

Considering the above restrictions, only four studies qualify as applicable to sprays. Tong and Wang [10] studied particle laden 3D mixing layers under the assumption of one-way coupling. The particles are initially released in the upper stream and perturbations of the initial flow velocity profile induces roll-up of the layer, entrainment and mixing. It is found that specific 3D features evolve, such as many small-scale structures in the rib plane containing spanwise vorticity of both signs, and mushroom-like structures in the crosstream-spanwise plane. These structures effectively determine the local distribution of particles through the relative magnitude of the enstrophy and the square of the strain rate: while the rib vorticity induces ejection of particles, local straining induces particle accumulation. Unfortunately, no statistical analysis of the flow or particle field is presented that could lead to the development of SGS models. An enlarged investigation displaying essentially the same physics is also presented in [41]. Ling et al. [42] conducted a similar study of incompressible shear layers with one-way coupling and found that particles with a Stokes number of order unity had the largest concentration on the circumference of streamwise two-dimensional large scale structures forming in the flow. Similar to the results in [10] and [41], it was found that the variation of the particle concentration in both the spanwise and crosstream directions increases with the development of three-dimensional small scales structures, resulting in the mushroom-like shape of the particle distribution. It is though unclear if the simulations were pursued to turbulence transition, although the lack of internal small structures inside the large scale vortices suggests that the flow remained pre-transitional.

To this author's knowledge, the only study of 3D compressible shear layer with two-way coupling and phase change where transition to turbulence was achieved is due to Miller and Bellan [43]. The results show not only a preferential concentration of particles at the circumference of the large scale structures, but also a complex particle distribution inside these vortices due to the formation of the small scale turbulent structures. Whereas in the pre-transitional study [16] the droplets were shown to be ejected from the high vorticity fluid and to congregate in high strain regions due to their inertia through the preferential concentration mechanism, effectively mapping both the primary spanwise and streamwise structures (the 'focusing' effect discussed by Ling et al. [42]), the transitional state is considerably more complex. Although the number density contours are still indicative of preferential concentration, this occurs on a much smaller scale than in the pre-transitional state. Modulation of the flow by the particles occurs with increasing mass loading as the rotational energy of the final time flows is increased by the droplets due to both direct vorticity production and to additional disturbance wavelengths introduced by the coupling source terms. As Re^0 increases, the concentration field shows a mix of characteristics seen in [16] and those observed in other DNS of solid particle dispersion in isotropic turbulence. Increasing droplet mass loading ratios at fixed Re^0 was shown to produce a more 'natural' turbulence with lesser influences of the forcing perturbations on the long time flow fields, whereas increasing the initial Reynolds number at fixed mass loading promoted drop clustering. Subgrid analysis of the turbulent state was performed to study the effects of subgrid Eulerian gas phase variables as they affect the individual droplet transport, and a SGS model based on an extension of the eddy interaction model was developed for both the gas velocity and thermodynamic subgrid fluctuations to be used in future LES. This aspect of modeling is important; it was illustrated how neglecting these effects can lead to substantial errors in the droplet drag force, the droplet heating and the evaporation rates in LES. Also, the SS model of Liu et al. [25] was extended to predict the subgrid variances of all necessary LES variables. When based on a filter width dependent model constant, the SS model was shown to be reasonably accurate in capturing the variance behavior at both the Eulerian grid points and also at the droplet locations based on interpolations. A different model to account for the subgrid variance, and SGS constant coefficients based on the GR and SS models were proposed by Okong'o and Bellan [24], while dynamic SGS models are in progress [44]. Once satisfying *a posteriori* LES tests (to be performed in future work), these models have the potential for accurate spray simulations

Modeling issues for two-phase flow LES

From the above discussion, it appears that there are several issues that have so far been unresolved for LES spray simulations. One of these issues is the simulation of dense sprays which is discussed elsewhere in this volume [45]; we note that indeed all DNS/LES investigations so far address only the dilute spray regime. To account for drop interactions otherwise than with already modeled turbulence (e.g. Harstad and Bellan [46]), one would derive equations in the same manner as Drew [23], solve the ensemble averaged equations in a DNS, extract SGS models from the DNS database, filter the DNS equations to obtain the LES equations, replace the correlations in the LES equations by the SGS model, and solve the LES equations thus obtained. Although the concept is straightforward, implementing it is a considerable task which currently has not been undertaken for the realistic case of heating and evaporating drops. Other issues that have been briefly discussed above, are now discussed in more detail below.

Unfiltered values of variables at drop locations

As mentioned above, it is very important to have in a LES a model of the unfiltered variables at the drop locations because they affect all notable drop properties. So far, there are two such models available. In the model of Miller and Bellan [43] the subgrid variance is found by interpolating modeled variances from the Eulerian grid points to the local droplet locations and then employing a random number generator to produce 'assumed' Gaussian distributed fluctuations for all of the variables. Each droplet then interacts with these fluctuations for its 'eddy residence time' obtained from its relative duration spent within the subgrid filter width, $\Delta/|v_i|$, where v_i is the i^{th} component of the drop velocity. The assumption of Gaussian subgrid PDFs was tested with the DNS database and found to be adequate throughout most of the mixing layer, despite the fact that the ensemble of subgrid fluctuations are highly intermittent. The exception to this observation is the vapor mass fraction subgrid PDF, which shows substantial deviations from Gaussian behavior near the edges of the layer.

In the model of Okong'o and Bellan [24] each dependent variable φ is considered to be the sum of the filtered variable and a correction whose sign and magnitude must be found. Geometrical considerations combined with a Taylor series approximation of $O(\Delta^4)$ lead to the conclusion that the sign of the correction will be -*sign*$(\nabla^2\varphi)$. However, since it is not φ but the filtered value, $\overline{\varphi}$, which is available in the LES, the assumption is made that $\nabla^2\varphi$ and $\nabla^2(\overline{\varphi})$ have the same sign. Additional considerations and analysis lead to the conclusion that the magnitude of the correction is $\sqrt{\overline{\varphi\varphi}} - \sqrt{\overline{\overline{\varphi}\,\overline{\varphi}}}$. When this combined representation is tested against the database [43], it is found that all thermodynamic variables are approximated to better than 0.4%, whereas the velocities are within 1% of the unfiltered values. This accuracy was achieved for the case with the highest Re^0

at a state where the Reynolds number based on the momentum thickness was 1400, corresponding to a turbulent transitional state.

These two models offer different possibilities to investigators, according to the needs of the problem to be solved. Other representations might exist, and it would be helpful for the sake of future LES studies to build a library of such models that have been tested against databases.

SGS fluxes and subgrid variances

To this author's knowledge the only two-phase anisotropic, inhomogeneous flow DNS study considering drop heating and evaporation is that of Miller and Bellan [16], [43]. The subsequent study of Okong'o and Bellan [24] is therefore the first and only existing investigation concomitantly developing SGS models for the stresses, the heat and the species fluxes in the presence of evaporating drops. These fluxes of momentum, heat and species $\tau_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j$, $\theta_j = \widetilde{T u_j} - \widetilde{T}\widetilde{u}_j$, $\eta_j = \widetilde{Y_V u_j} - \widetilde{Y_V}\widetilde{u}_j$, respectively, naturally appear in the LES equations once the third and fourth order correlations have been approximated by second order correlations using the DNS database as an assessment tool. Together with these fluxes, the subgrid variance σ_{SGS} must also be evaluated. Noting that generically $\sigma^2_{SGS} = \overline{\varphi\varphi} - \overline{\varphi}\,\overline{\varphi}$, it is immediately apparent that the subgrid variance has the same form as the fluxes, and this is what prompted Okong'o and Bellan [24] to model them in the same manner using the GR and SS models. The GR model was found to give excellent results when the modeling constant is properly calculated using the database [24], whereas the SS model was also found accurate when the modeling constant was calculated using a test to grid filter ratio of 2 [24] which is the value recommended by investigators of single-phase flows.

LES source terms

One important remaining question is the modeling of the averaged source terms in the LES equations. In the context of the Eulerian/Lagrangian representation this is equivalent to inquiring what is the number of real drops that can be replaced by a 'computational' drop. Therefore, in the LES Eulerian/Lagrangian formalism, the drop equations should be considered to represent computational rather than real drops. We note that calculations making this approximation have already been performed (e.g. Mostafa and Mongia [47]) but without the advantage of the rigorous evaluation that can be made during a DNS/LES study. This evaluation is currently in progress.

In the context of the Eulerian/Eulerian representation the issue of number of drops followed is moot since the drop number density equation is solved [10]. The equivalent issue becomes the appropriate averaged representation of terms such as $Pe_c^{-1} \times \nabla^2 n$, $Pe_c^{-1} \times \nabla^2 \overrightarrow{u}$, $Pe_c^{-1} \times \nabla^2 Y_V$ and $Pe_c^{-1} \times \nabla^2 T$ where Pe_c is based on an effective diffusivity, κ_c. The magnitude of κ_c is appropriately chosen so that in the DNS calculation the drop number density equation is well resolved (imposing a lower bound on κ_c) while at the same time insuring the local aspect of the averaging (imposing an upper bound on κ_c). The introduction of this local diffusivity is conceptually similar to a local diffusive smoothing in the Eulerian/Lagrangian method with the exception that the smoothing is an operation that is performed after the drop equations have been solved, whereas the effective local diffusion is applied as the equations are being solved. Miller and Bellan [16] have used a locally conservative instead of a locally diffusive smoothing and have shown that the local drop number density is grid dependent when the grid spacing is larger than the interdrop distance. It is the averaged drop number density that is the truly physical and measurable quantity, paralleling the situation in molecular theory [48]. Since n is defined in [10] as the drop number density above an inner scale, it already represents an average and it is in this context that its magnitude must be understood. Because in an Eulerian/Eulerian formalism the equations are typically solved at the same scale for carrier flow and particles, the carrier flow dependent variables must be defined at the same inner scale. Particular care should then be devoted to define all these scales prior to initiating the DNS/LES protocol to insure that the results are meaningful and that the LES grid filter is chosen consistently for drops and flow. To this author's knowledge, such a DNS/LES study has not yet been performed.

Conclusions

The state-of-the-art in LES studies relevant to sprays has been here reviewed. The survey showed that there is a remarkable small number of studies addressing the combination of crucial phenomena needed for the accurate description of sprays, i.e. anisotropy, inhomogeneity and three-dimensionality at the small scale, without appealing to strictly single-phase SGS models. Although both the Eulerian/Lagrangian and Eulerian/Eulerian approaches have been pursued, the former is at a considerably more advanced stage of development. Four important issues have been identified which remain at the stage of work in progress: the simulation of DNS/LES for dense sprays, the modeling of the interaction of the small scale turbulence with the drops, the modeling of the SGS stresses, heat and species fluxes, and the modeling of the source terms in the LES equations. These issues must all be resolved prior to attempting an LES calculation. Even if these issues are resolved, it is not certain that the resulting LES will yield a stable calculation due to the coupling between the large and small scales that is inherently missing in the procedure for developing SGS models. Further work is needed in all these areas before one could confidently simulate sprays in an accurate manner.

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